ABSTRACT OF THE DISCLOSURE

Provided herein are computer-based methods for generating and using three-dimensional (3-D) structural models of target molecules and databases containing the models. The targets can be protein structural variants derived from genes containing polymorphisms. The models are generated using molecular modeling techniques and are used in structure-based drug design studies for identifying drugs that bind to particular structural variants in structure-based drug design studies, for designing allele-specific drugs and population-specific drugs and for predicting clinical responses in patients. Computer-based methods for predicting drug resistance or sensitivity via computational phenotyping are also provided. Databases containing protein structural variant models are also provided.